

Spin-orbit coupling in Fe-based superconductors

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Abstract We study the spin resonance peak in recently discovered iron-based superconductors. The resonance peak observed in inelastic neutron scattering experiments agrees well with predicted results for the extended s -wave (s_{\pm}) gap symmetry. Recent neutron scattering measurements show that there is a disparity between longitudinal and transverse components of the dynamical spin susceptibility. Such breaking of the spin-rotational invariance in the spin-liquid phase can occur due to spin-orbit coupling. We study the role of the spin-orbit interaction in the multiorbital model for Fe-pnictides and show how it affects the spin resonance feature.

Keywords Fe-based superconductors · Spin-resonance peak · Spin-orbit coupling

The nature of the superconductivity and gap symmetry and structure in the recently discovered Fe-based superconductors (FeBS) are the most debated topics in condensed matter community [1]. These quasi two-dimensional systems shows a maximal T_c of 55 K placing them right after high- T_c cuprates. Fe d -orbitals form

the Fermi surface (FS) which in the undoped systems consists of two hole and two electron sheets. Nesting between these two groups of sheets is the driving force for the spin-density wave (SDW) long-range magnetism in the undoped FeBS and the scattering with the wave vector \mathbf{Q} connecting hole and electron pockets is the most probable candidate for superconducting pairing in the doped systems. In the spin-fluctuation studies [2, 3, 4], the leading instability is the extended s -wave gap which changes sign between hole and electron sheets (s_{\pm} state) [5].

Neutron scattering is a powerful tool to measure dynamical spin susceptibility $\chi(\mathbf{q}, \omega)$. It carries information about the order parameter symmetry and gap structure. For the local interactions (Hubbard and Hund's exchange), χ can be obtained in the RPA from the bare electron-hole bubble $\chi_0(\mathbf{q}, \omega)$ by summing up a series of ladder diagrams to give $\chi(\mathbf{q}, \omega) = [I - U_s \chi_0(\mathbf{q}, \omega)]^{-1} \chi_0(\mathbf{q}, \omega)$, where U_s and I are interaction and unit matrices in orbital space, and all other quantities are matrices as well.

Scattering between nearly nested hole and electron Fermi surfaces in FeBS produce a peak in the normal state magnetic susceptibility at or near $\mathbf{q} = \mathbf{Q} = (\pi, 0)$. For the uniform s -wave gap, $\text{sign} \Delta_{\mathbf{k}} = \text{sign} \Delta_{\mathbf{k}+\mathbf{Q}}$ and there is no resonance peak. For the s_{\pm} order parameter as well as for an extended non-uniform s -wave symmetry, \mathbf{Q} connects Fermi sheets with the different signs of gaps. This fulfills the resonance condition for the interband susceptibility, and the spin resonance peak is formed at a frequency below $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{Q}}|)$ (compare normal and s_{\pm} superconductor's response in Fig. 1) [6, 7, 8]. The existence of the spin resonance in FeBS was predicted theoretically [6, 7] and subsequently discovered experimentally with many reports of well-defined spin resonances in 1111, 122, and 11 systems [9, 10, 11].

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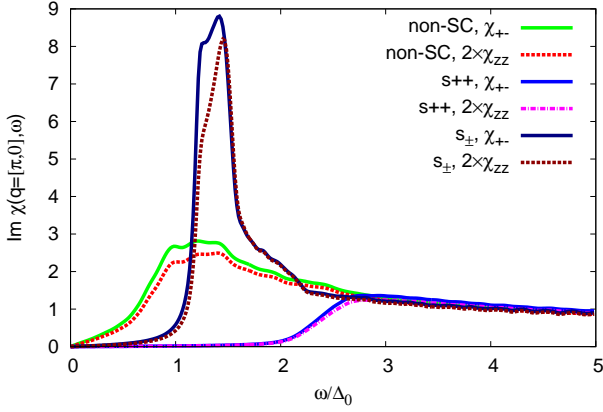


Fig. 1 Fig. 1. Calculated $\text{Im}\chi(\mathbf{Q}, \omega)$ in the normal state, and for the s_{++} and s_{\pm} pairing symmetries. In the latter case, the resonance is clearly seen below $\omega = 2\Delta_0$. Spin-orbit coupling constant $\lambda = 100$ meV, intraorbital Hubbard $U = 0.9$ eV, Hund's $J = 0.1$ eV, interorbital $U' = U - 2J$, and pair-hopping term $J' = J$.

One of the recent puzzles in FeBS is the discovered anisotropy of the spin resonance peak in Ni-doped Ba-122 [12]. It was found that χ_{+-} and $2\chi_{zz}$ are different. This contradicts the spin-rotational invariance (SRI) $\langle S_+ S_- \rangle = 2 \langle S_z S_z \rangle$ which have to be obeyed in the disordered system. One of the solution to the puzzle is the spin-orbit (SO) interaction which can break the SRI like it does in Sr_2RuO_4 [13]. Here we incorporate the effect of the SO coupling in the susceptibility calculation for FeBS to shed light on the spin resonance anisotropy.

The simplest model for pnictides in the 1-Fe per unit cell Brillouin zone comes from the three t_{2g} d -orbitals. The xz and yz components are hybridized and form two electron-like FS pockets around $(\pi, 0)$ and $(0, \pi)$ points, and one hole-like pocket around $\Gamma = (0, 0)$ point. The xy orbital is considered to be decoupled from them and form an outer hole pocket around Γ point. The one-electron part of the Hamiltonian is given by $H_0 = \sum_{\mathbf{k}, \sigma, l, m} \epsilon_{\mathbf{k}}^{lm} c_{\mathbf{k}l\sigma}^\dagger c_{\mathbf{k}m\sigma}$, where l and m are orbital indices, $c_{\mathbf{k}m\sigma}$ is the annihilation operator of a particle with momentum \mathbf{k} and spin σ . This model for pnictides is similar to the one for Sr_2RuO_4 and, in particular, the xy band does not hybridize with the xz and yz bands. Keeping in mind the similarity to the Sr_2RuO_4 case, for simplicity we consider only the L_z -component of the SO interaction [13]. Due to the structure of the L_z -component, the interaction affects xz and yz bands only.

Following Ref. [14], we write the SO coupling term, $H_{SO} = \lambda \sum_f \mathbf{L}_f \cdot \mathbf{S}_f$, in the second-quantized form as

$H_{SO} = i\frac{\lambda}{2} \sum_{l, m, n} \epsilon_{lmn} \sum_{\mathbf{k}, \sigma, \sigma'} c_{\mathbf{k}l\sigma}^\dagger c_{\mathbf{k}m\sigma'} \hat{\sigma}_{\sigma\sigma'}^n$, where ϵ_{lmn} is the completely antisymmetric tensor, indices $\{l, m, n\}$ take values $\{x, y, z\} \leftrightarrow \{d_{yz}, d_{zx}, d_{xy}\} \leftrightarrow \{2, 3, 1\}$, and $\hat{\sigma}_{\sigma\sigma'}^n$ are the Pauli spin matrices.

The matrix of the Hamiltonian $H = H_0 + H_{SO}$ is then

$$\hat{\epsilon}_{\mathbf{k}\sigma} = \begin{pmatrix} \epsilon_{1\mathbf{k}} & 0 & 0 \\ 0 & \epsilon_{2\mathbf{k}} & \epsilon_{4\mathbf{k}} + i\frac{\lambda}{2}\text{sign}\sigma \\ 0 & \epsilon_{4\mathbf{k}} - i\frac{\lambda}{2}\text{sign}\sigma & \epsilon_{3\mathbf{k}} \end{pmatrix} \quad (1)$$

As for Sr_2RuO_4 , eigenvalues of $\hat{\epsilon}_{\mathbf{k}\sigma}$ do not depend on spin σ , therefore, spin-up and spin-down states are still degenerate in spite of the SO interaction.

We calculated both $+-$ (longitudinal) and zz (transverse) components of the spin susceptibility and found that in the normal state $\chi_{+-} > 2\chi_{zz}$ at small frequencies, see Fig. 1. As expected, for the s_{++} superconductor (conventional isotropic s -wave) there is no resonance peak and the disparity between χ_{+-} and $2\chi_{zz}$ is very small. For the s_{\pm} superconductor, however, the situation is opposite – we observe a well defined spin resonance and χ_{+-} is larger than $2\chi_{zz}$ by about 15% near the peak position (Fig. 1).

In summary, we have shown that the spin resonance peak in FeBS gains anisotropy in the spin space due to the spin-orbit coupling. This result is in qualitative agreement with experimental findings. We do not observe changes in the peak position but this may be due to the simple model that we studied.

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